
ACCURACY OF AN ALGEBRAIC SUB-STRUCTURING METHOD FOR LARGE-SCALE EIGENVALUE COMPUTATION

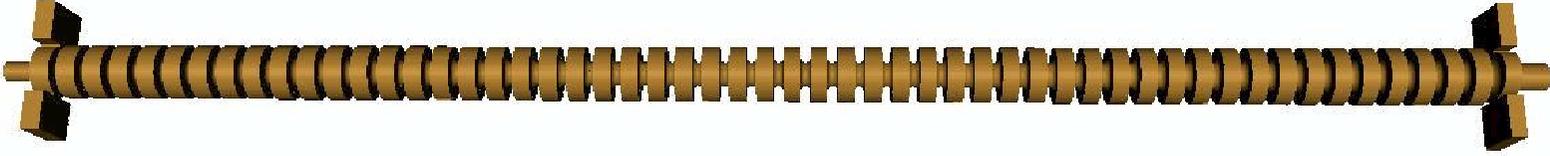
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Introduction

- Electromagnetic simulation of next generation accelerator design (SciDAC)



- Modeled by Maxwell's equations

$$\begin{aligned}\Delta \times (\Delta \times \mathbf{E}) - \lambda \mathbf{E} &= 0 && \text{in } \Omega, \\ \mathbf{n} \times \mathbf{E} &= 0 && \text{on electric boundary } \Gamma_E, \\ \mathbf{n} \times (\Delta \times \mathbf{E}) &= 0 && \text{on magnetic boundary } \Gamma_B\end{aligned}$$

- A hierarchical vector finite elements discretization scheme leads to a very large generalized eigenvalue problem

$$Kx = \lambda Mx$$

Sub-structuring

- Basic idea: solving a large problem by breaking it into few smaller sub-structures.
- Common technique for the static/dynamic properties of large engineering structures.
- An automated multi-level sub-structuring (AMLS) method has been successfully applied for vibration and acoustic analysis of large FEM problems, and is significantly faster than conventional approaches [Bennighof *et al.*].
- Our goal: examine the accuracy of sub-structuring methods for large-scale eigenvalue computation from an algebraic point of view.

$S = \text{diag}(S_1, S_2, I)$, S_i contains a few eigenvectors of (K_{ii}, M_{ii}) , computed in parallel!

$$(S^T \widehat{K} S)^q = \theta (S^T \widehat{M} S)^q \xrightarrow{\text{projection}} \widehat{K} = \begin{pmatrix} K_{11} & & \\ & K_{22} & \\ & & K_{33} \end{pmatrix}, \quad \widehat{M} = \begin{pmatrix} M_{11} & & \\ & M_{22} & \\ & & M_{13}^T \quad \widehat{M}_{13}^T \quad \widehat{M}_{23} \quad \widehat{M}_{33} \end{pmatrix}$$

↑ congruent transform

$$Kx = \lambda Mx \xleftarrow{\text{reordering}} \widetilde{K} = \begin{pmatrix} K_{11} & & \\ & K_{22} & \\ & & K_{13} \quad K_{23} \quad K_{33} \end{pmatrix}, \quad \widetilde{M} = \begin{pmatrix} M_{11} & & \\ & M_{22} & \\ & & M_{13}^T \quad M_{23}^T \quad M_{33} \end{pmatrix}$$

Algebraic sub-structuring method

How many eigenvectors of submatrices to select?

- S_1 and S_2 consist of only a few eigenvectors of subproblems.
- Central questions: what and how many eigenmodes of sub-structures to compute?
- Answer: A new selection criterion is to choose those eigenmodes of sub-structures such that

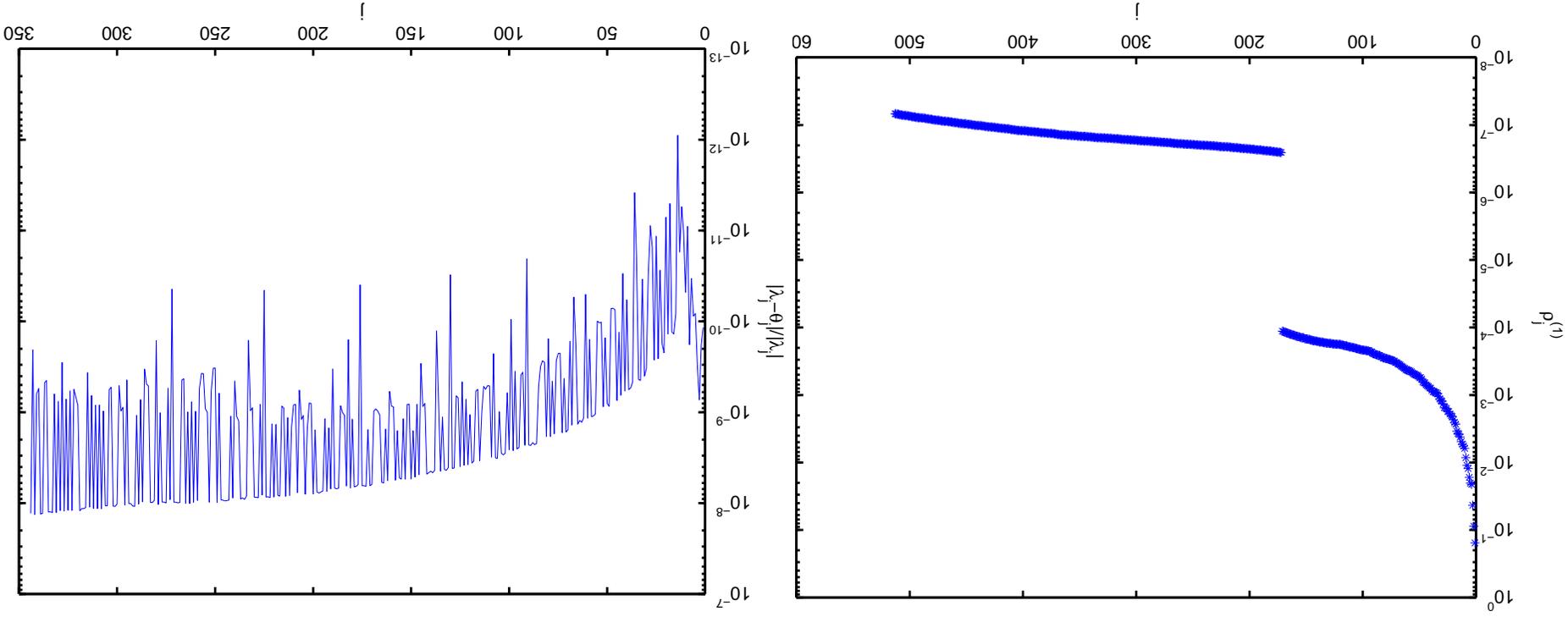
$$p_k(\lambda_j^{(i)}) \leq \tau = \text{threshold},$$

where $\lambda_j^{(i)}$ are the eigenmodes of sub-structure i ,

$$p_k(\omega) = \left| \frac{\omega - \lambda_k}{\lambda_k} \right|,$$

and λ_k is the desired eigenvalue of (K, M) .

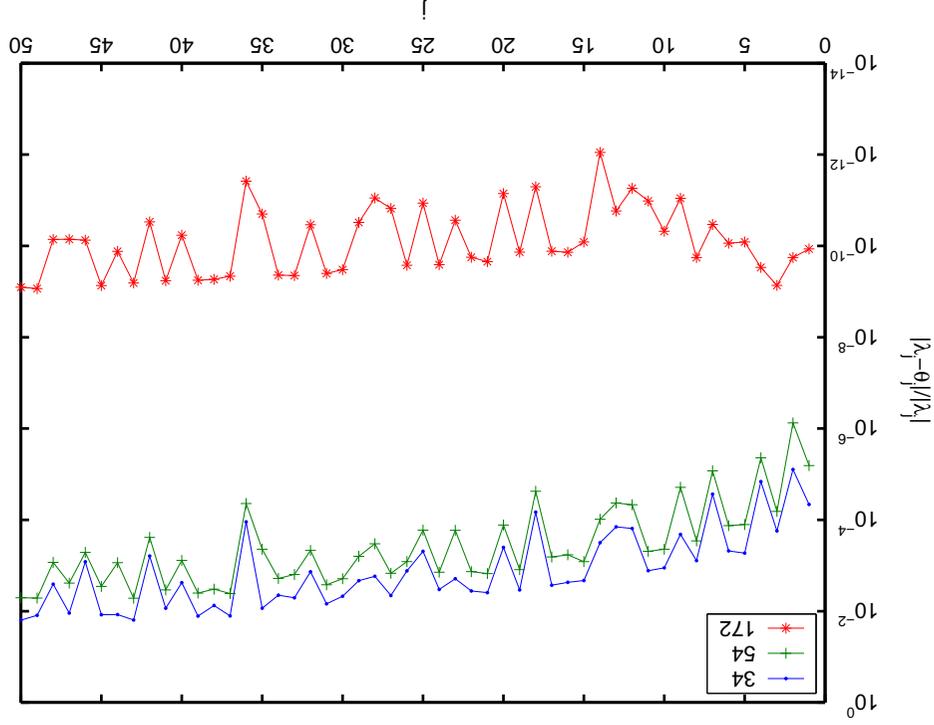
Case study I: BCSTK, M09



$p_1^{(i)}(\lambda_j^{(i)})$ and the relative error of the approximate eigenvalues with 172 eigenvectors from each subproblem.

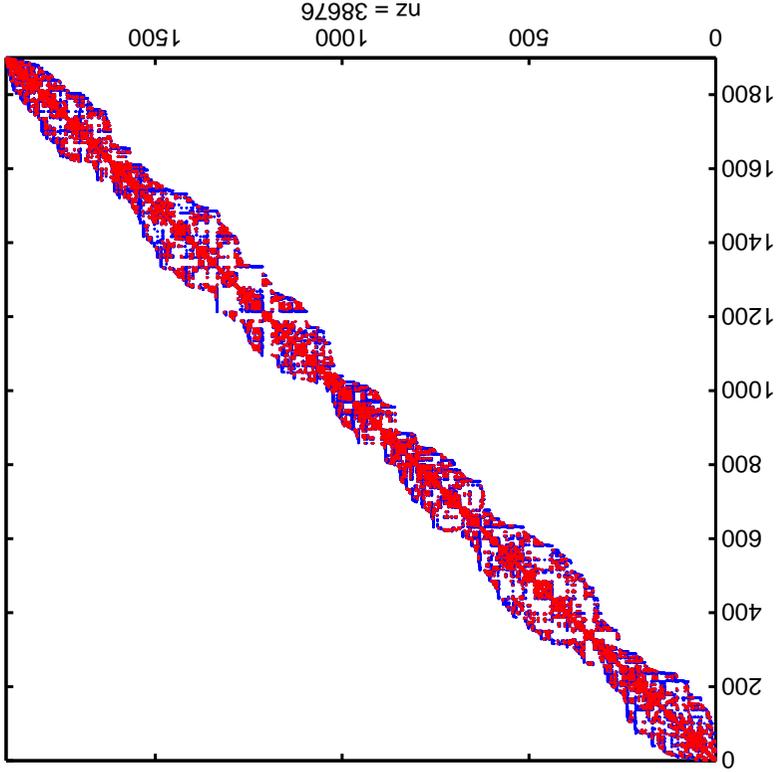
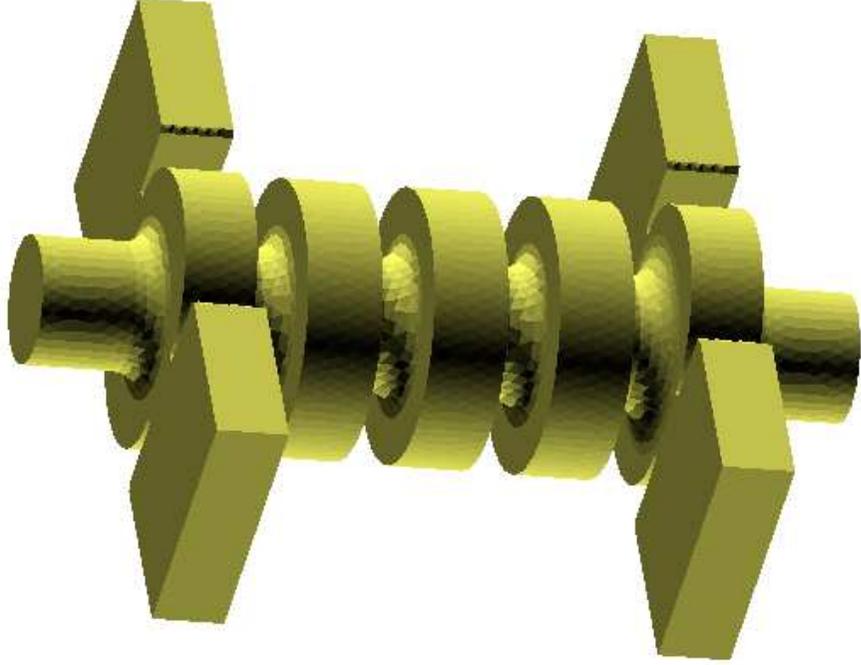
Case Study I: Impact of threshold τ

- The relative error of the smallest 50 eigenvalues of (K, M) .



- 34 and 54 approximate eigenvalues are obtained by setting the threshold to 10^{-3} and 5×10^{-4} respectively.
- 172 approximate eigenvalues are obtained by setting the threshold to 10^{-6} .

Case Study II: Short traveling wave accelerating structure



5-cell traveling wave accelerating structure and sparsity of FEM matrices K and M .

Case Study II: Null space deflation

- Hierarchical vector finite element discretization leads to singular K . Deflation is necessary.

- The generalized eigenvalue problem is of the form

$$\begin{pmatrix} K_{11} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda \begin{pmatrix} M_{11} & M_{12}^T \\ M_{12} & M_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

We are only interested in the non-zero eigenvalues and the corresponding eigenvectors.

- Applying a modified nested dissection reordering to $K + M$ to separate null spaces of sub-structures:

$$K_{ii} = \begin{pmatrix} A_i & 0 \\ 0 & 0 \end{pmatrix}, \quad M_{ii} = \begin{pmatrix} B_i & C_i^T \\ C_i & D_i \end{pmatrix},$$

where A_i contains only non-zero rows and columns of K_{ii} and nonsingular.

- The congruent transform is then defined by

$$T^{-1} = \begin{pmatrix} I_{n_1} & & & \\ & I_{n_2} & & \\ & & -K_{13}^T K_{11}^\dagger & \\ & & -K_{23}^T K_{22}^\dagger & \\ & & & I_{n_3} \end{pmatrix} \text{ where } K_{ii}^\dagger = \begin{pmatrix} A_{-1}^i & & \\ & 0 & \\ & & 0 \end{pmatrix}$$

- The non-zero eigenvalues and the corresponding eigenvectors of each sub-structure

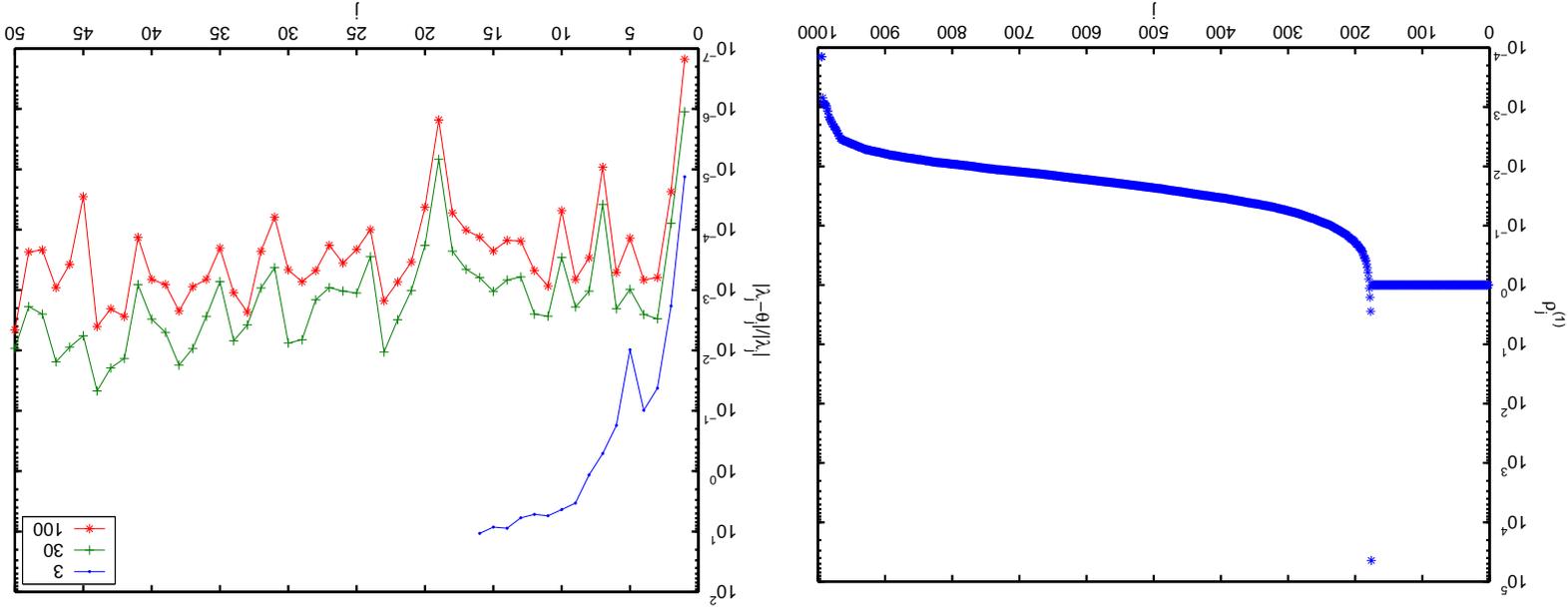
are computed from the reduced problem

$$A^i q = \lambda^{(i)} (B^i - C_i^T D_i^{-1} C_i) q.$$

- The projected eigenvalue problem is

$$\begin{pmatrix} \tilde{K}_{11} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \theta \begin{pmatrix} \tilde{M}_{11} & \tilde{M}_{12}^T \\ \tilde{M}_{12} & \tilde{M}_{22} \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}.$$

Case Study II: Mode selection and accuracy



The p -factor and the relative error of the approximate eigenvalues.

- 5 digits accuracy of the smallest non-zero eigenvalue if only 3 eigenvalues from each sub-structure.
- With the threshold $\tau = 10^{-1}$ (10^{-2}), 30 (100) eigenvalues are selected from each sub-structure. The relative error of smallest 50 eigenvalues are all below 10^{-2} (10^{-3}).

Concluding remarks and future work

- We have a better understanding of the accuracy of the algebraic substructuring method for large scale eigenvalue computation.
- An efficient null space deflation scheme is designed and is extendable to multi-level substructures.
- Future work includes:

- A practice way to select the most important modes from each sub-structure in the absence of a full decomposition of sub-structure.
- An efficient method to solve a large number of nonzero eigenvalues in the presence of a large null space.
- Preconditioning techniques, such as the development of a congruent transform to make clustered spectral components of interest.